

NASA TT F-11,493

A QUANTUM MECHANICAL THEORY OF ADSORPTION OF INERT GAS  
ATOMS ON A SOLID SURFACE

Motoaki Sugawara

Translated from "Kokugakkaishi" (Journal of the  
Aeronautical Society of Japan)  
Vol. 13, No. 139, pp. 266-270, (August 1965)

FACILITY FORM 602

**N68-17739**  
(ACCESSION NUMBER)

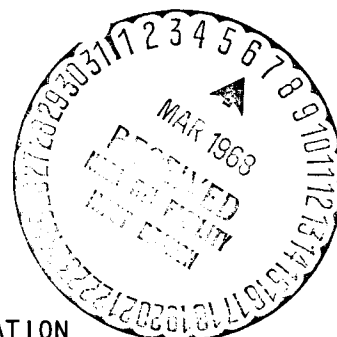
(PAGES) 1

(NASA CR OR TMX OR AD NUMBER) 1

(THRU) \_\_\_\_\_

(CODE) 23

(CATEGORY) \_\_\_\_\_



NATIONAL AERONAUTICS AND SPACE ADMINISTRATION  
WASHINGTON, D. C. 20546

FEBRUARY 1968

A QUANTUM MECHANICAL THEORY OF ADSORPTION OF INERT GAS  
ATOMS ON A SOLID SURFACE

M. Sugawara

ABSTRACT: Calculations are made on the probability of trapping an inert gas atom on a solid surface. A linear lattice is taken as a model for the solid crystal. The interaction potential between the solid surface and a gas atom is assumed to be the square well type. For every energy level of the bound state, there exists an incident energy which has the maximum probability of trapping.

This paper discusses previous research and experimentation on the boundary conditions on the surface of a solid in a stream of low density gas and describes a method of quantum mechanical calculation of them, postulating a simple collision model for the interaction of gas and solid molecules.

/266\*

### 1. Introduction

One of the problems remaining in the dynamics of rarefied gases is that of boundary conditions, as described in "Prospects." This problem is also important in calculating the flow of an actual gas, as Takano has described elsewhere in this issue. It is impossible to determine accurate boundary conditions unless one knows clearly at what velocity and in which direction a gas molecule (atom), which strikes the surface of a solid in a certain direction and velocity, is reflected. In the past, this problem has been investigated by dividing it into two approaches. In one approach, the problem is restricted to one dimension and the difference between the velocity of the incident gas molecule and the velocity of the reflected gas molecule is described, i.e. a thermal accommodation coefficient is determined. The other approach is to determine the law of distribution of the angles of reflection. Experiments and theoretical studies on the former approach have been conducted for a long time, but the first highly reliable work began in 1930 with the publication of the results of experiments by J. K. Roberts [1].

In the 1930's, British physicists, primarily J. M. Jackson, N. F. Mott, A. Howarth, J. E. Lennard-Jones, C. Strachan and A. F. Devonshire published a series of reports to explain the results of Robert's experiments [2, 9]. Their approach is to consider a solid as an aggregate of many oscillators, to determine the probability of transition of the state of oscillation of the oscillators in the solid when struck by a gas atom and to derive the thermal

---

\* Numbers in the margin indicate pagination in the foreign text.

accommodation coefficient from this. Since they consider that the incident gas atom strikes the surface of the solid perpendicularly, no information concerning angular distribution can be obtained. Moreover, they give no consideration to the process in which part of the kinetic energy of the incident atom is absorbed by the surface of the solid and is transmitted to the inside.

Consequently, no explanation is given concerning the trapping of the gas atom by the solid surface after the atom has lost its kinetic energy, i.e., the process occurring when adsorption is taking place. Physicists lost interest in the problem of the interaction of gas molecules and solid surfaces after the 1930's, and no one considered the problem again until the end of the 1950's. However, at that time, after the launching of artificial satellites, it became necessary to determine the coefficient of resistance of an object flying through rarefied gas. At that time, attention again became focused on the interaction of gas molecules and solid surfaces, and many experiments were conducted concerning measurement of the thermal accommodation coefficient, and the distribution of incident molecules and incident angles. At the present time at least, the experiment data are almost all available [10]. However, no progress has been made on the theoretical side since the series of papers written in the 1930's. In particular, no theory exists concerning the incident angle distribution.

The difficulty with any theory of reflected angle distribution arises from the fact that, especially in the vicinity of normal temperatures, there is apparently mixing of diffuse reflection and specular reflection, since a considerable amount of incident molecules (atoms) are ejected after being adsorbed momentarily on the solid surface (See Figure 1). For this reason, it is first necessary to explain, from the standpoint of mechanics, the mechanism

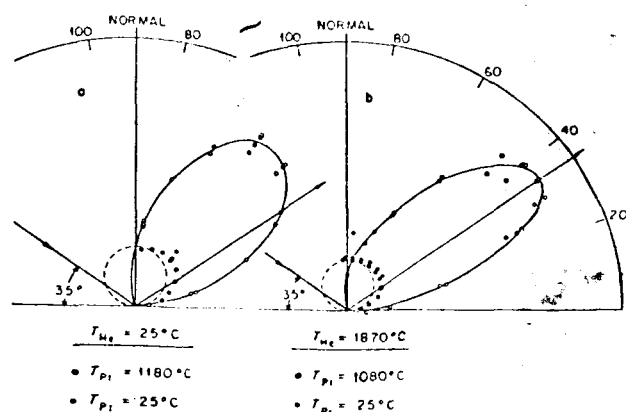


Figure 1. Angular Distribution of Helium Reflected from Platinum Surface (See Reference 10).

of adsorption, in order to construct a valid theory of reflected angle distribution. Classical mechanical calculations of this were carried out recently by B. M. McCarroll and G. Ehrlich [11] for a one-dimensional chain type crystal model. However, their calculations are only for the case where the temperature of the solid is absolute zero. This is due to the difficulty of giving an initial vibration corresponding to the temperature, in one-dimensional chain type crystals.

However, adsorption has been considered as a phenomenon occurring on a quantum mechanical scale, so the author presents quantum mechanical calculations on a one-dimensional model.

## 2. The Model

/267

The solid is considered to be a chain of atoms of mass  $M$ , distributed at equal intervals on a straight line. In the transmission of energy in such a model, the excitation of a state of vibration in some atoms causes a state of vibration in other atoms, due to their interaction, i.e. this takes place in the form of the transport of phonons. If we disregard the interaction occurring between atoms other than those adjoining each other, the process of generation and extinction of phonons due to their collision does not occur in the one-dimensional model [12]. In such a case, the solution of Boltzmann's equation expressing the transport of phonons is expressed in the form  $N = \text{func}(z - vt)$ , where  $N$  is the number of phonons in a wave packet at position  $z$ . This expresses a traveling wave proceeding at a velocity  $v$ , without changing its shape.

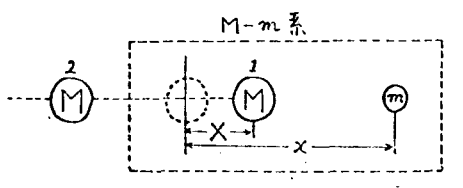


Figure 2. M-m System.

Now we consider the case of a gas atom of mass  $m$  striking in one dimension in the direction of the chain of solid atoms (See Figure 2). We consider here only two atoms: the gas atom and the atom on the surface of the solid (atom No. 1 in the figure), and call this system M-m. Henceforth the atoms on the surface and the gas atoms will be called  $M$  and  $m$ , respectively. The instant that atom  $m$  strikes atom  $M$  is assumed to be  $t = t_0$ . Assuming that

$N$  phonons are generated at the moment of collision in atom  $M$  (atom 1) which sustained the collision of atom  $m$ ; these  $N$  phonons all move to atom 2 when  $t = t_0 + a_0/v$  (where  $v$  here is the rate of propagation of the phonons, and  $a_0$  is the distance between lattices in the solid crystal). That is, energy of  $N\hbar\omega$  is lost from system M-m. (Here,  $\hbar$  is the value obtained by dividing the Planck constant by  $2\pi$  and  $\omega$  is the angular oscillation frequency when  $M$  is assumed to be a harmonic oscillator). However, it is not possible to determine the process occurring while energy is being discharged from system M-m, when  $t$  is within  $t_0 \sim t_0 + a_0/v$ , from the solution of Boltzmann's equation which does not contain the term for collision. For this reason we make the following assumptions.

There is no loss of energy from system M-m when  $t < t_0 + a_0/2v$

Energy loss is  $N\hbar\omega$  from system M-m when  $t > t_0 + a_0/2v$ .

### 3. Schroedinger's Equation and Its Solution

Using the above assumption, Schroedinger's equation for system M-m can be written as follows:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} + \frac{1}{2} M \omega^2 X^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, X) - N\hbar\omega E \left\{ t - \left( t_0 + \frac{a_0}{2v} \right) \right\} \right] \psi \quad (1)$$

Here,  $\psi$  is the wave function of system M-m,  $V(x, X)$  is the potential energy from the interaction of M and m. The coordinates  $X, x$  indicate respectively, the positions of atoms M and m with the equilibrium point of atom M as the origin (See Figure 2). Also,  $E \left\{ t - \left( t_0 + \frac{a_0}{2v} \right) \right\}$  is the unit function determined by the following equation:

$$E \left\{ t - \left( t_0 + \frac{a_0}{2v} \right) \right\} = \begin{cases} 0 & t < t_0 + \frac{a_0}{2v} \\ 1 & t > t_0 + \frac{a_0}{2v} \end{cases}$$

Now, the energy discharge from system M-m, which is expressed by the last term in equation (1), occurs suddenly when  $t = t_0 + a_0/2v = t_1$ . At this instant, the wave function itself may be considered as unchanging. Expressing the wave function when  $t < t_1$  as  $\psi_1$ , and as  $\psi_2$  when  $t > t_1$ , we assume these can be expressed as follows by the wave functions of unperturbed systems  $\chi_{mn}(x, X)$  and  $\pi_{kl}(x, X)$ . /268

$$\left. \begin{aligned} t < t_1: \psi_1 &= \sum_{m,n} a_{mn}(t) \chi_{mn}(x, X) e^{-\frac{i}{\hbar} (W_m + E_n)t} \\ t > t_1: \psi_2 &= \sum_{k,l} b_{kl}(t) \pi_{kl}(x, X) e^{-\frac{i}{\hbar} (W_k + E_l)t} \end{aligned} \right\} \quad (2)$$

The specific forms of  $\chi$  and  $\pi$  are indicated later. The symbol  $\sum$  indicates integration of energy eigenvalues when the energy eigenvalues  $E_n, W_n, E_l, W_k$  are continuous. If there are any discrete ones, it indicates the sum with respect to their eigenvalues. Now, since when  $t = t_1, \psi_1 = \psi_2$ ,

$$\begin{aligned} & \sum a_{mn}(t_1) \chi_{mn}(x, X) e^{-\frac{i}{\hbar} (W_m + E_n)t_1} \\ &= \sum b_{kl}(t_1) \pi_{kl}(x, X) e^{-\frac{i}{\hbar} (W_k + E_l)t_1} \end{aligned}$$

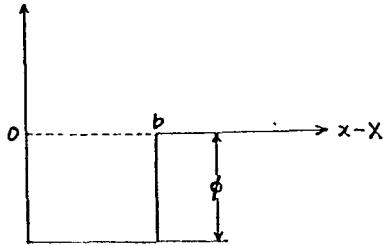
Multiplying both sides by  $\pi_{pq}^*$  and integrating over all coordinates,

$$b_{pq}(t_1) = \sum a_{mn}(t_1) \left[ \iint \pi_{pq}^* \chi_{mn} dx dX \right] \times \exp \left\{ -\frac{i}{\hbar} (W_m + E_n) t_1 + \frac{i}{\hbar} (W_p + E_q') t_1 \right\} \quad (3)$$

is obtained. Here  $\pi_{k1}$  is assumed to satisfy the normalized condition

$$\iint \pi_{k1}^* \pi_{k1} dx dX = 1$$

As is indicated below, the equation expressing  $b_{pq}(t)$  includes one constant of integration and is determined by the conditions in (3). Now, let us determine some concrete forms of  $\psi_1$  and  $\psi_2$ . For this purpose, the interaction potential  $V(x, X)$  must be given. We assume the form of  $V(x, X)$  to be as follows (See Figure 3).



$$V = \begin{cases} 0 & x-X > b \\ -\phi & 0 < x-X < b \\ \infty & x-X < 0 \end{cases}$$

Figure 3. Interaction Potential.

Equation (1) is solved for such  $V(x, X)$ , but here we will solve using a perturbation method [13]. Basically  $V$  is a function of  $(x - X)$ , but since  $X$  is small we assume it to be close to zero, and considering  $V$  to be a function only of  $x$ , we will rewrite as follows:

$$V(x) = \begin{cases} 0 & x > b \\ -\phi & 0 < x < b \\ \infty & x < 0 \end{cases}$$

First, we shall determine the wave function  $\psi_1$ , when  $t < t_1$ . For a zero order approximation equation of equation (1), the following equation is obtained:

$$i\hbar \frac{\partial \phi}{\partial t} = \left[ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} + \frac{1}{2} M \omega^2 X^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \phi \quad (4)$$

Separation of variables is possible in equation (4), so its solution can be expressed by

$$\begin{aligned}(\psi_0)_{mn} &= f_m(x) g_n(X) e^{-\frac{i}{\hbar} (W_m + E_n)t} \\ &= \chi_{mn}(x, X) e^{-\frac{i}{\hbar} (W_m + E_n)t}\end{aligned}$$

where we assume  $\chi_{mn}(x, X) = f_m(x) g_n(X)$ , and  $f_m(x)$ ,  $g_n(X)$  are eigenfunctions satisfying, respectively, the following equations:

$$\begin{aligned}\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right] f_m(x) &= W_m f_m(x) \\ \left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} + \frac{1}{2} M \omega^2 X^2\right] g_n(X) &= E_n g_n(X)\end{aligned}$$

The  $W_m$ ,  $E_n$  in the above equations are eigenvalues of the operators on the left side and are usually called energy eigenvalues. Now, we assume that the correct solution of equation (1) is expressed by

$$\psi_1 = \sum_{m,n} a_{mn}(t) (\psi_0)_{mn} \quad (5)$$

Substituting (5) and (1), the following equation is obtained for the expansion coefficient  $a_{mn}$ .

$$\begin{aligned}i\hbar \dot{a}_{rs}(t) e^{-\frac{i}{\hbar} (W_r + E_s)t} \\ = \sum_{m,n} a_{mn}(t) e^{-\frac{i}{\hbar} (W_m + E_n)t} \left[ \iint \chi_{rs}^* V' \chi_{mn} dx dX \right]\end{aligned}$$

Here  $V'$  is the perturbation potential

$$V' = V(x - X) - V(x),$$

and  $\chi_{mn}$  is assumed to be normalized. Assuming the expansion coefficient of  $(t < 0)$  before interaction takes place to be  $a_{mn}(0)$ , the expansion coefficient  $a_{rs}$  at time  $t$  becomes as follows, through approximation

$$\begin{aligned}a_{rs}(t) &= a_{rs}(0) - \sum_{m,n} \frac{a_{mn}(0)}{W_m + E_n - W_r - E_s} \\ &\quad \times \left\{ 1 - e^{-\frac{i}{\hbar} (W_m + E_n - W_r - E_s)t} \right\} \\ &\quad \times \iint \chi_{rs}^* V' \chi_{mn} dx dX\end{aligned} \quad (6)$$

The probability  $P_{rs}$  that the particle expressed as a wave packet will be detected in state  $rs$  at time  $t$  is given by the following equation.

$$P_{rs} = |a_{rs}(t)|^2 \quad (7)$$

However, this refers to the case where  $t < t_1$ .

It is also possible to determine the wave function  $\psi_2$  where  $t > t_1$  in the same manner as follows:

$$\psi_2 = \sum_{k,l} b_{kl}(t) (\phi'_0)_{kl} \quad \underline{/269}$$

Here,

$$\begin{aligned} (\phi'_0)_{kl} &= f_k(x) u_l(X) e^{-\frac{i}{\hbar}(W_k + E_l')t} \\ &= \pi_{kl}(x, X) e^{-\frac{i}{\hbar}(W_k + E_l')t} \end{aligned}$$

$f_k(x)$  belongs to the same system of functions as  $f_m(x)$  as in the case of  $\psi_1$  and  $u_1(X)$  is the eigenvalue satisfying the following equation.

$$\left[ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} + \frac{1}{2} M \omega^2 X^2 - N \hbar \omega \right] u_l(X) = E_l' u_l(X)$$

assuming that  $\pi_{k1}(x, X) = f_k(x) u_1(X)$  is normalized, the expansion coefficient  $b_{k1}(t)$  is expressed approximately as follows [14]:

$$\begin{aligned} b_{pq}(t) &= b_{pq}(t_1) + \sum_{k,l} \frac{b_{kl}}{(W_k + E_l' - W_p - E_q')} \\ &\times \left\{ e^{-\frac{i}{\hbar}(W_k + E_l' - W_p - E_q')t} \right. \\ &\quad \left. - e^{-\frac{i}{\hbar}(W_k + E_l' - W_p - E_q')t_1} \right\} \\ &\times \iint \pi_{pq}^* V' \pi_{kl} dx dX \end{aligned}$$

Assuming that  $t$  and  $t_1$  are not much different from what they were in equation (3), the following relationship is obtained.

$$|b_{pq}(t)|^2 = |a_{pq}(t_1)|^2$$

The significance of this is that the probability that system M-m will be found in state  $b_{pq}$  is equal to  $|a_{pq}(t_1)|^2$ . Consequently, the values of  $P_{rs}$  in equation (7) where  $t = t_1$  express the probability after  $t_1$ . To find

$P_{rs}$  from equation (7), it is necessary to find the values in the following equation which are called matrix elements

$$V'_{rs.mn} = \iint \chi_{rs}^* V' \chi_{mn} dx dX \quad (8)$$

Since we are dealing with the phenomenon of adsorption, we may assume  $W_m > 0$ ,  $W_r < 0$ . For purposes of further simplification, the state of oscillation of atom M is first the basic state ( $n = 0$ ), so let us consider the case in which it collides with atom m and changes to the first state of excitation ( $n = 1$ ). Of course, the state of oscillation of atom M is not limited to  $n = 0$ . The transition occurring from collision is not restricted to  $0 \rightarrow 1$ , as there is also  $0 \rightarrow 2$ ,  $0 \rightarrow 3$ , etc., but we shall consider here only  $0 \rightarrow 1$ , whereupon  $f_m$ ,  $f_r$ ,  $g_0$ ,  $g_1$  become respectively, as follows:

$$f_m(x) = \begin{cases} c \sin \alpha x & (0 < x < b) \\ \left( c \sin \alpha b \cdot \sin \beta b + c \frac{\alpha}{\beta} \cos \alpha b \cos \beta b \right) \sin \beta x \\ + \left( c \sin \alpha b \cdot \cos \beta b - c \frac{\alpha}{\beta} \sin \beta b \cos \alpha b \right) \\ \times \cos \beta x & (b < x) \end{cases} \quad (9)$$

$$f_r(x) = \begin{cases} c' \sin \alpha' x & (0 < x < b) \\ c' e^{\beta' b} \sin \alpha' b \cdot e^{-\beta' x} & (b < x) \end{cases} \quad (9')$$

Here

$$\alpha = \sqrt{\frac{2m(W_m + \phi)}{\hbar^2}}, \quad \beta = \sqrt{\frac{2m W_m}{\hbar^2}}$$

$$\alpha' = \sqrt{\frac{2m(\phi - |W_r|)}{\hbar^2}}, \quad \beta' = \sqrt{\frac{2m |W_r|}{\hbar^2}}$$

Also,  $c$ ,  $c'$  are determined by normalized conditions.

$$g_0 = \frac{r^{1/2}}{\pi^{1/4}} e^{-\frac{1}{2} r^2 X^2}, \quad g_1 = \frac{\sqrt{2} r^{3/2}}{\pi^{1/4}} \times e^{-\frac{1}{2} r^2 X^2}$$

Here,

$$r = \sqrt{\frac{M\omega}{\hbar}}$$

Substituting each of the above equations in (8)

$$\begin{aligned}
V'_{r1,m0} &= \phi \int_{-\infty}^0 \frac{\sqrt{2} r^2}{\sqrt{\pi}} \times e^{-r^2 X^2} dX \int_{x+b}^b f_r f_m dx \\
&\quad - \phi \int_0^{\infty} \frac{\sqrt{2} r^2}{\sqrt{\pi}} \times e^{-r^2 X^2} dX \int_b^{x+b} f_r f_m dx \\
&\approx -\frac{\sqrt{2} \phi}{2r} c c' \sin \alpha' b \cdot \sin \alpha b
\end{aligned} \tag{10}$$

is obtained. An extremely troublesome procedure of approximation computations is required until the final equation in (10) is obtained and is omitted here.

#### 4. Procedure Using Wave Packet

According to equation (7), the incident wave packet must first be given in order to determine the probability that the particle will be found in a trapped state. This is because the energy eigenvalues of the final (trapped) state are rather scattered, so that it is not possible to derive the transition probability per unit of time, which is normally not a function of time, and even if the incident particle is expressed by a plane wave, significant results cannot be obtained. The wave packet which originally should have been given included the two variables  $x$ ,  $X$ , but since the state of oscillation of the solid atom is clearly indicated for both prior and after interaction,  $x$  and  $X$  can be separated and the incident particle alone can be expressed by the wave packet. The wave packet expressing the incident particle where  $t = 0$ , is given such that it has the given average velocity and average position  $x = b$ . Any form of the wave packet will do, but it cannot be expanded by eigenfunctions (9) and (9') unless it is zero when  $x = 0$  and  $x = L$  ( $L$  is the length used when the eigenfunction of the incident particle has been normalized). Consequently, the generally employed minimum wave packet [13]

$$\Psi(x) = [2\pi(\Delta x)^2]^{-1/4} \exp \left[ -\frac{(x - \langle x \rangle)^2}{4(\Delta x)^2} + i \frac{\langle p \rangle}{\hbar} x \right]$$

cannot be employed. (In the above equation,  $\langle x \rangle$  and  $\langle p \rangle$  are average values for position and momentum respectively,  $\Delta x$  is the uncertainty of the position). The author attempted to find  $a_{rs}(t)$  by following equation (6), for a wave packet with several simple shapes, but at the stage of determining the expansion coefficient  $a_{mn}(0)$  in the case when the given wave packet where time  $t = 0$  was expanded by the energy eigenfunctions (9) and (9'), it was necessary to determine many definite integrals, so the numerical computations were performed on Tokyo University's OKITAC 5090, but the capacity of the computer was somewhat too small and adequate results were not obtainable. I would like to postpone specific examples of numerical values to a later report. However, the following conditions can be seen from equations (6) and (10). The matrix elements in equation (10) may become zero, according to the value of kinetic energy  $W_m$  of the incident particle, and in this case, the  $a_{rs}(t)$  computed by equation (6) approaches zero.

/270

Consequently, practically no adsorption occurs in this case. For example, using tungsten for atom M and helium for atom m, using the numerical values of

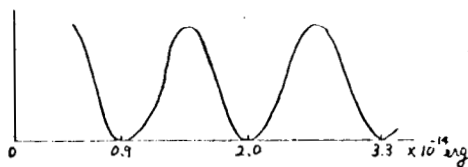


Figure 4. Probability of Adsorption Being Caused.

$b = 5 \times 10^{-8}$  cm,  $\phi = 8.54 \times 10^{-14}$  erg,  $\omega = 2.7 \times 10^{13}$  rad/s,  $a_0 = 3 \times 10^{-8}$  cm,  $v = 5.4 \times 10^{-5}$  cm/s, the matrix element becomes zero, where  $W_m$  is  $0.9 \times 10^{-14}$  erg.,  $2.0 \times 10^{-14}$  erg,  $3.3 \times 10^{-14}$  erg,

so in this vicinity, the adsorption probability approaches zero (See Figure 4). However, Figure 4 is an estimation.

#### Acknowledgements

In writing this report, I should like to express my sincere thanks to Prof. Kondo Jiro and Asst. Prof. Tanaka Akira of the Aeronautics Department of Tokyo University, and to my colleagues in Dr. Kondo's laboratory, for their guidance and assistance.

#### REFERENCES

1. Roberts, J. K.; The Exchange of Energy Between Gas Atoms and Solid Surface; Proc. Roy. Soc., Vol. A129, pp. 146-161, 1930.
2. Jackson, J. M.; A Quantum Mechanical Theory of Energy Exchange Between Inert Gas Atoms and a Solid Surface; Proc. Camb. Phil. Soc.; Vol. 28, pp. 136-164, 1932.
3. Jackson, J. M. and N. F. Mott; Energy Exchange Between Inert Gas Atoms and a Solid Surface; Proc. Roy. Soc., A 137, p. 703, 1932.
4. Jackson, J. M. and A. Howarth; Exchange of Energy Between Inert Gas Atoms and a Solid Surface; Proc. Roy. Soc.; Vol. A 142, pp. 447-456; 1933.
5. Lennard-Jones and Strachan; The Interaction of Atoms and Molecules with Solid Surfaces I.; Proc. Roy. Soc.; Vol. A 150; p. 442, 1935.
6. Strachan, C.; The Interaction of Atoms and Molecules with Solid Surfaces II; Proc. Roy. Soc., Vol. A156, p. 456, 1935.
7. Lennard-Jones, J. E. and A. F. Devonshire; The Interaction of Atoms and Molecules with Solid Surfaces III; Proc. Roy. Soc.; Vol. A 156 p. 6, 1936.
8. Devonshire, A. F.; The Interaction of Atoms and Molecules with Solid Surfaces VIII; Proc. Roy. Soc., Vol. A 158, p. 269, 1937.
9. Strachan, C.; The Interaction of Atoms and Molecules with Solid Surfaces IX, Proc. Roy. Soc., Vol. A 158, p. 591, 1937.

10. Laurmann, J. A.; Rarefied Gas Dynamics, Vol. I; Academic Press, New York, 1963.
11. McCarroll, B. and G. Ehrlich; Trapping and Energy Transfer in Atomic Collisions with a Crystal Surface; Jour. Chem. Phys., Vol. 38, Number 2, 1963.
12. Pyles (Translator Usui Tsunemaru, *et. al.*), Quantum Theory of Solids, p. 49, Yoshioka Press.
13. Shiff (Translator Inoue Ken) Quantum Mechanics I, Yoshioka Press.
14. Shinichiro, Asanaga; Quantum Mechanics II, p. 282, Misuzu Shobo Press.
15. American Institute of Physics; American Institute of Physics Handbook; McGraw-Hill Press.

Translated for the National Aeronautics and Space Administration under Contract No. NASw-1695 by Techtran Corporation, P. O. Box 729, Glen Burnie, Maryland, 21061.